LCA Case Studies

Modeling Process and Material Alternatives in Life Cycle Assessments*

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Abstract

Background, Aims and Scope. Although LCA is frequently used in product comparison, many practitioners are interested in identifying and assessing improvements *within* a life cycle. Thus, the goals of this work are to provide guidelines for scenario formulation for process and material alternatives within a life cycle inventory and to evaluate the usefulness of decision tree and matrix computational structures in the assessment of material and process alternatives. We assume that if the analysis goal is to guide the selection among alternatives towards reduced life cycle environmental impacts, then the analysis should estimate the inventory results in a manner that: (1) reveals the optimal set of processes with respect to minimization of each impact of interest, and (2) minimizes and organizes computational and data collection needs.

Methods. A sample industrial system is used to reveal the complexities of scenario formulation for process and material alternatives in an LCI. The system includes 4 processes, each executable in 2 different ways, as well as 1 process able to use 2 different materials interchangeably. We formulate and evaluate scenarios for this system using three different methods and find advantages and disadvantages with each. First, the single branch decision tree method stays true to the typical construction of decision trees such that each branch of the tree represents a single scenario. Next, the process flow decision tree method strays from the typical construction of decision trees by following the process flow of the product system, such that multiple branches are needed to represent a single scenario. In the final method, disaggregating the demand vector, each scenario is represented by separate vectors which are combined into a matrix to allow the simultaneous solution of the inventory problem for all scenarios.

Results. For both decision tree and matrix methods, scenario formulation, data collection, and scenario analysis are facilitated in two ways. First, process alternatives that cannot actually be chosen should be modeled as sub-inventories (or as a complete LCI within an LCI). Second, material alternatives (e.g., a choice between structural materials) must be maintained within the analysis to avoid the creation of artificial multi-functional processes. Further, in the same manner that decision trees can be used to estimate 'expected value' (the sum of the probability of each scenario multiplied by its 'value'), we find that expected inventory and impact results can be defined for both decision tree and matrix methods.

Discussion. For scenario formulation, naming scenarios in a way that differentiate them from other scenarios is complex and important in the continuing development of LCI data for use in databases or LCA software. In the formulation and assessment of scenarios, decision tree methods offer some level of visual appeal and the potential for using commercially available software/ traditional decision tree solution constructs for estimating expected values (for relatively small or highly aggregated product systems). However, solving decision tree systems requires the use of sequential process scaling which is difficult to formalize with mathematical notation. In contrast, preparation of a demand matrix does not require use of the sequential method to solve the inventory problem but requires careful scenario tracking efforts.

Conclusions. Here, we recognize that improvements can be made within a product system. This recognition supports the greater use of LCA in supply chain formation and product research, development, and design. We further conclude that although both decision tree and matrix methods are formulated herein to reveal optimal life cycle scenarios, the use of demand matrices is preferred in the preparation of a formal mathematical construct. Further, for both methods, data collection and assessment are facilitated by the use of sub-inventories (or as a complete LCI within an LCI) for process alternatives and the full consideration of material alternatives to avoid the creation of artificial multi-functional processes.

Recommendations and Perspectives. The methods described here are used in the assessment of forest management alternatives and are being further developed to form national commodity models considering technology alternatives, national production mixes and imports, and point-to-point transportation models.

Keywords: Decision trees; expected value; inventory analysis; material choice; process choice

Introduction

Often, when building a life cycle inventory, process and material alternatives are relevant throughout the life cycle. For example, a fuel cell power plant for the production of electricity can mean the inclusion of upstream processes for the production of hydrogen or natural gas, consideration of heat recovery or the exhaust of waste heat, and the disposal or recycling of steel, graphite, and/or ceramic components. Selection among the alternatives can reveal an improved system. Thus, there is a focus here on process and material alternatives **within** a life cycle inventory (LCI) and opportunities to improve or optimize the system.

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Extensive research has focused on inventory optimization. Notably, Azapagic and Clift provide not only a review of methods and applications but also additional implementation details [1–3]. Their overall method begins with a contribution analysis for a baseline Life Cycle Assessment (LCA) which is used to identify 'hot spots' in the system where alternatives should be considered. Next, these authors use multi-objective optimization as the basis for identifying the optimal system. Here, we provide additional information on scenario formulation and data management and evaluate the usefulness of decision tree and matrix computational structures in the assessment of material and process alternatives. We assume that if the goal of an analysis is to guide the selection among alternatives towards reduced life cycle environmental impacts, then the analysis should estimate the inventory results in a manner that: (1) reveals the optimal set of processes with respect to minimization of each impact of interest, and (2) minimizes and organizes computational and data collection needs.

Existing methods for scenario formulation and evaluation are decision tree analysis, disaggregation of the demand vector, process aggregation, and statistical simulation:

1. **Scenario or decision tree analysis.** Decision trees have long been used in the economic analysis of industrial systems [4, 5] and more recently in data mining [6, 7] and countless other applications. Similarly, Heijungs and Suh [8] cite Morgan and Henrion [9] who suggest the use of scenario or decision trees in LCA. As demonstrated in Bage [10, 11], this method uses "scenario trees with qualitative levels to study the propagation of uncertainties due to the process alternative chosen." By 'qualitative levels,' Morgan and Henrion mean that the scenario trees have multiple levels of decisions each with their own probabilities and values.
2. **Disaggregation of the demand vector.** In an LCI, the demand vector represents the reference flow or the amount of product demanded by the economic system of interest to fulfill the functional unit. In Heijungs and Suh's mathematical formulation, the demand vector is used with the technology matrix A (representing all flows within the technosphere or flows between unit processes within the system boundaries) to estimate scaling factors s or the amount of each unit process needed to meet the system demand (such that $s=A^{-1}f$). Disaggregation of the demand vector allows comparison of system alternatives through the preparation of a demand matrix **f** (combining vectors as f_1, f_2, etc.) so that a scaling matrix **s** (denoted as s_1, s_2, etc.) represents separate solutions to the inventory problem.
3. **Process aggregation.** In this method, process alternatives are aggregated into a single process whose flows are weighted averages of all process alternatives by the percentage of market share or the probability that each alternative is applied. This method is often used in modeling the 'electricity grid' for regions or countries. However, Heijungs and Suh note that technology probability measures can be very difficult to obtain for the wide variety of process technologies modeled within an inventory. Further, aggregation of process alternatives does not facilitate selection between alternatives when such selection is possible.
4. **Statistical simulation.** Heijungs and Suh again cite Morgan and Henrion who suggest the use of Monte Carlo simulations based on probability distributions. However, Heijungs and Suh also describe process alternatives as a 'discrete choice' that, unlike other uncertainties in LCA, cannot be described in terms of Gaussian distributions. Within that context, there is only one mention of multi-modal distributions by Morgan and Henrion. They state it is easier to see multi-modal distributions with a probability density function than it is with a cumulative distribution function. However, they note that "It is generally easier to express probabilistic dependencies among variables as discrete conditional probability distributions, than to express them in terms of correlations between continuous variables."

It is important to note that material alternatives in a scenario can occur with or without process alternatives. For example, whereas alternative pesticides can be used in crop production with no other changes in that unit process, the use of liquid carbon dioxide or siloxane (D5) in dry cleaning requires different equipment and energy and ancillary material flows than systems using perchloroethylene. Material alternatives can be modeled as process alternatives by, for example, recording material differences in the process name: one might name the unit process for dry cleaning as 'dry cleaning using perchloroethylene,' 'dry cleaning using liquid carbon dioxide,' and 'dry cleaning using siloxane.'

Noting that the use of aggregation of all process and material alternatives and Monte Carlo simulations do not allow sufficient differentiation between alternatives in situations in which such a choice can be made, further investigation of decision tree analysis and disaggregation of the demand vector are presented here.

1 Example Product System with Process and Material Alternatives

Consider for example the product system presented in the *process flow diagram* in **Fig. 1**, displaying only flows within the technosphere (flows between unit processes within the system boundaries) and not including for example energy production and transport. As shown, P_A is the process that produces material A and processes P_{B1} or P_{B2} can be used to produce material B. Materials A and B are then used in P_C to produce material C. Next, material C is used in P_{F1} or P_{F2} to produce material F. Finally, material F is combined with material D or E produced in P_{D1} or P_{D2} or P_{E1} or P_{E2} in the final process which creates the end product. In summary, Fig. 1 includes:

1. **Process alternatives.** A set of processes that produce the same product using different methods. Process alternatives are designated by P_{mi} where m is the type of product produced and i is an index for the alternatives in the set. There are 4 processes each with 2 process alternatives in Fig. 1: P_{B1} or P_{B2}; P_{D1} or P_{D2}; P_{E1} or P_{E2}; and P_{F1} or P_{F2}.
2. **Material alternatives.** A set of materials that can be used interchangeably in a specific unit process. There is one material alternative in Fig. 1: the use of material D or E in the production of the end product.

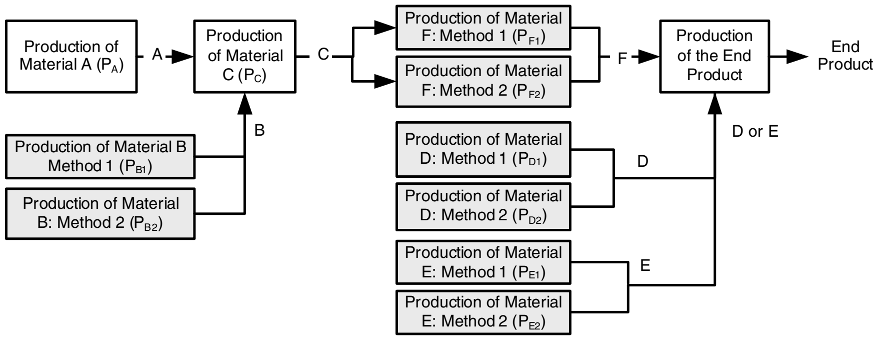

Fig. 1: Process flow diagram for the example product

The example system includes 7 processes (P_A– P_F and P_{EP}, 4 of which have 2 alternatives) and 6 materials (A–F, 1 of which has 2 alternatives: process P_{EP} can use material D or E) resulting in 16 unique systems or scenarios to be evaluated.

Further consideration of the example product system reveals two critical issues: (1) each time consideration of an alternative is added to an LCA, the data collection, management, and assessment requirements increase and (2) the ability to actually choose between alternatives may not span the entire life cycle. For the latter, a product designer is able to specify the use of recycled as opposed to virgin materials but may not be able to dictate the use of only renewable energy sources in materials production nor whether or not the product user actually recycles the final product. Thus, an opportunity exists to investigate mathematical system reduction methods that include only viable decisions among process and material alternatives. Thus, an assessment of decision tree and disaggregated demand vector analyses as applied to the example product system follows.

2 Decision Tree Methods

LCA practitioners can use decision trees to formulate and evaluate scenarios for process and material alternatives. As suggested by Heijungs and Suh [8], decision trees can be used to prepare scenarios in an organized fashion while still maintaining relationships between the parameters. In addition, decision trees allow the practitioner to differentiate between decisions that can be made and chances or probabilities for which there is no control. Despite these advantages within the context of LCA, Heijungs and Suh provide little information on the use of scenario or decision trees in LCA and little research was found that implemented decision tree methods in the context of LCA. An exception is presented by Bage, et al. [10,11] who use decision tree analysis to determine the path that will provide an optimal solution in the remediation of contaminated sites. Their example lays out very distinct stages or 'qualitative levels' in the remediation of an example site and provides a mathematical basis to determine the optimal solution based on probabilities. These authors recognize that decisions made upstream affect the processes that occur after a decision is made and that there are only a limited number of choices that are under the decision-maker's control. However, their example does not address multiple decisions occurring concurrently and how decisions affect upstream processes. For example, in the product system depicted in Fig. 1, if Material D is chosen over Material E (a decision made relatively late in the life cycle) the upstream processes change where as in the work of Bage, et al., the decisions only affect subsequent life cycle processes.

To assess the impact of alternatives on both the up- and down-stream processes, two types of decision trees are developed here: (1) a **single branch decision tree** stays true to the typical construction of decision trees such that each branch of the tree represents a single scenario, and (2) a **process flow decision tree** which strays from the typical construction of decision trees by following the process flow of the product system such that multiple branches represent a single scenario. Each scenario includes a series of decisions and chances that reflect discrete choices among process and material alternatives that either can be made (e.g., design decisions such as will the product be made from aluminum or plastic) or cannot be influenced (e.g., chances such as whether a blast or electric arc furnace is used in steel production).

Fig. 2 presents a single branch decision tree assuming the *there is control* over the selection between P_{B1} and P_{B2}, between materials D and E, and between P_{E1} or P_{E2} but *must leave to chance* the use of P_{D1} or P_{D2} and the use of P_{F1} or P_{F2}. In keeping with typical development of decision trees, decisions are represented as boxes and chances are represented as circles. At each decision or chance node, the tree branches and new branches are added. Each branch must be followed through to the end product, with one scenario of the 16 possible highlighted in Fig. 2.

As shown in Fig. 2, if multiple materials enter into a unit process, the practitioner must represent these processes as sequential processes in order to keep each scenario a single branch. In the example, materials C and D are needed to create material F; however, when looking at the decision tree, it appears as if P_C is needed to produce an input to P_{D1} when in reality both P_C and P_{D1} feed directly into P_{F1}. This construction can be confusing to practitioners familiar with process flow diagrams but is necessary to allow the user to follow only one branch to the end of a scenario as is typical in decision tree construction.

The single branch method has a number of advantages and disadvantages. The fact that this method follows only one branch is its biggest advantage and when the number of unit

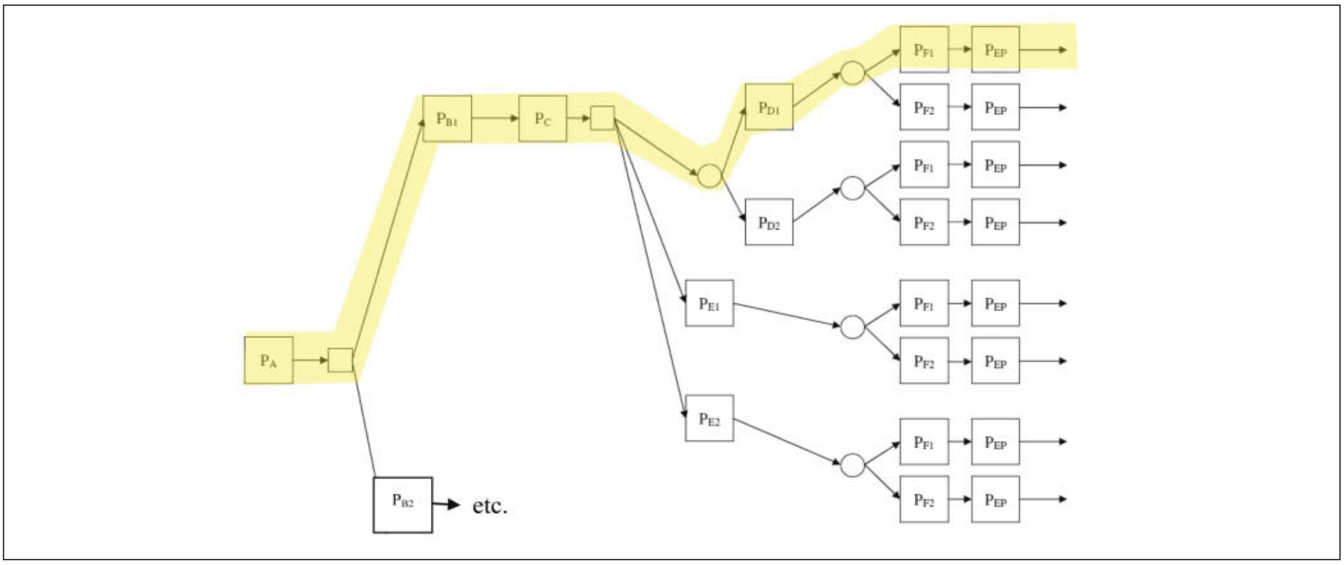

Fig. 2: Single branch decision tree

process and material alternatives are small this method might be the preferred method. Another advantage is that the method allows the use of readily available decision tree mathematical formulations and software, for the management and analysis of inventory data. However, the single branch method has a major disadvantage when looking at larger process systems: it gets very complicated very quickly. Because there is only one branch being followed for a single scenario all of the processes for all the materials must be in each branch, meaning that (1) each process alternative is repeated many times in the total tree and (2) the processes will not necessarily be in order of material and process flow causing confusion as which process is actually followed by the previous processes and which materials flow into which processes.

The process flow decision tree method was developed so that the flow of the processes and materials within the decision tree would appear intuitive to practitioners familiar with process flow diagrams. The decision tree is again developed from beginning to end. However, when processes require multiple inputs, a scenario must have multiple branches associated with it. **Fig. 3** shows an example process flow decision tree using the system defined above and highlighting the same scenario as is highlighted in Fig. 2.

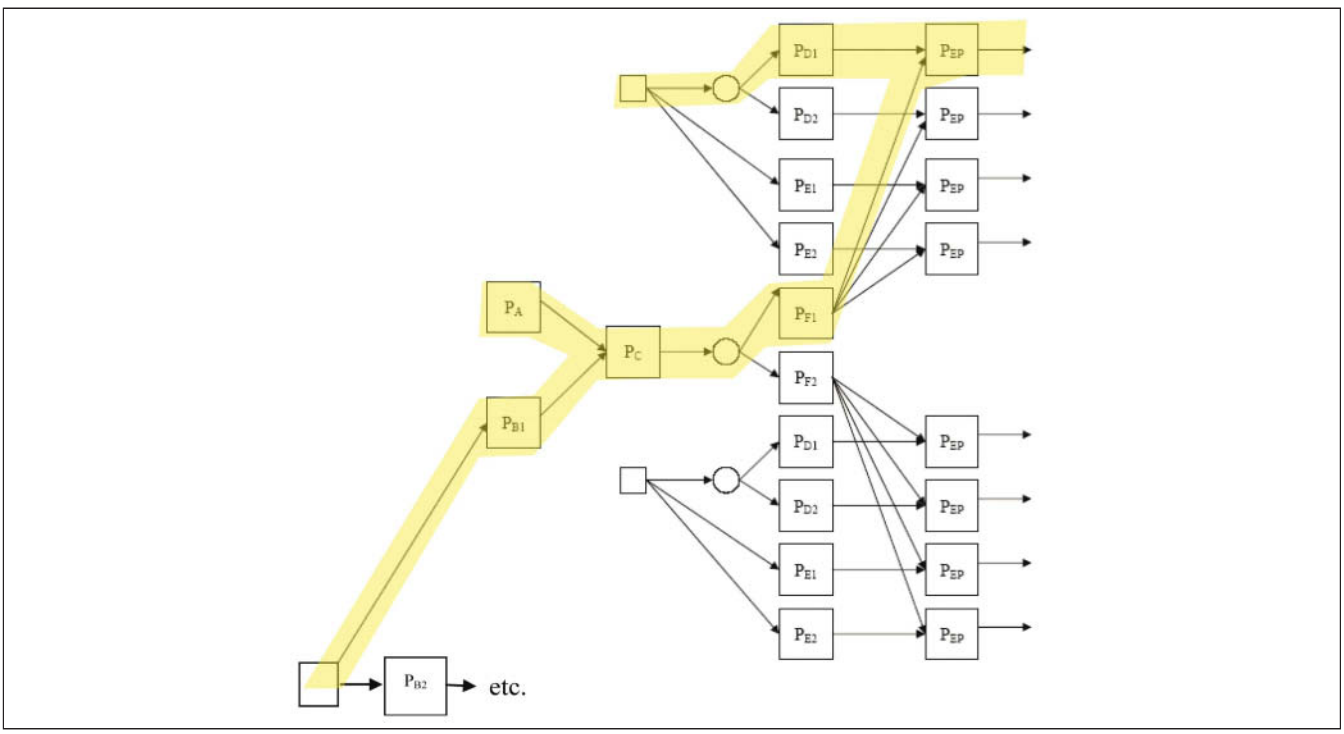

Fig. 3: Process flow decision tree

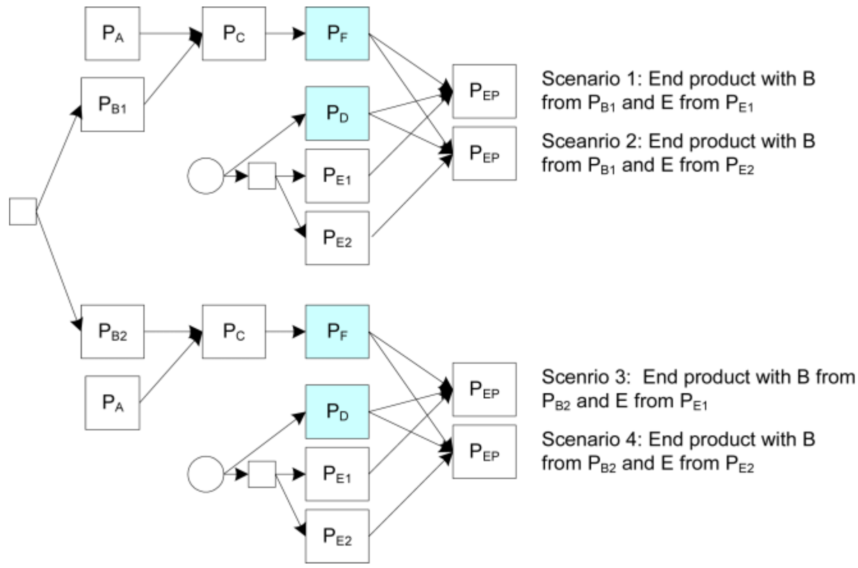

Fig. 4: Example product system with available process decision and material chance nodes (as a process flow decision tree)

The process flow decision tree method makes it easier to visually follow the actual flow of materials and processes while still showing the decisions and chances throughout. However, the practitioner must follow multiple branches to the end product and therefore cannot easily use decision tree software or solution methods to analyze the process tree. On the other hand, there is no confusion as to which materials flow into and out of each process because all processes are laid out in a way that also represents the material and process flows. Also, the tree again becomes quite complicated for large systems and decision tree software can not be used as designed to estimate the pay-off using the process-flow decision tree method.

Both the single branch method and the process flow method become very complicated when looking at large product systems. Because the decision trees get so much larger as the number of decisions and chances within the tree increase, the aggregation of process and material alternatives at chance nodes is investigated below to eliminate unavailable choices.

Again, aggregation of process and material alternatives can be based on market shares or the probability that the chosen technology is appropriate. Suppose, referring again to Fig. 1, that both the process and material alternatives are aggregated. For example, the production of materials D and F are aggregated such that P_{D1} and P_{D2} as well as P_{F1} and P_{F2} are combined to create one aggregate process P_D /P_F. Using either method, aggregating process and material alternatives reduces the number of scenarios from 16 to only 6. For both methods of aggregation, the decision trees better reflect what can be controlled within the life cycle. With larger systems this reduction will be even more substantial.

However, because there is not a unique process for the production of material D and F, the unit process P_D/P_F is multifunctional. Methods to address multifunctional processes are to use [8,12] system expansion, allocation, or the surplus method with the substitution method recommended by the ISO14040 standards as preferred. The partitioning and surplus methods can be used, for example, when there is no other way to produce the co-product than the process being modeled (i.e., no technology exists that can be called an avoided process), when computations 'snowball' when avoided processes are also multifunctional, or when there are significant differences in the quality of products. However, because system expansion and partitioning essentially require the disaggregation of the processes just aggregated, any simplification of the decision tree is lost.

Moving forward, we assume there is an advantage to aggregating process alternatives. We also assume the aggregation of material alternatives should be avoided. As a result, processes P_{D1} and P_{D2} are combined to form P_D and processes P_{F1} and P_{F2} are combined to form P_F. The system now includes 16 processes and 16 flows within the technosphere, with 4 unique scenarios depicted in **Fig. 4**. Thus, maintaining the 2 process alternatives (a choice between P_{B1} and P_{B2} and a choice between P_{E1} and P_{E2}) and the 1 material alternative (a 'chance' between materials D and E) dictates a need for 4 ways to produce the final product. Note that if the material alternative had been preceded by a decision node instead of a chance node, 6 unique scenarios would result.

Next, suppose additional processes are added to the system as depicted in **Fig. 5**. Specifically, suppose P_X, P_Y, and P_Z precede P_A; P_U, P_V, and P_W precede P_{B1}; P_Q, P_R, P_S and P_T precede P_{B2}; P_O and P_P precede P_C; P_N precedes P_F; P_M precedes P_{E2}; and P_L and P_K follow P_{E2}. In this case, 'sub-inventories' (or a complete LCI within an LCI) can be used to manage LCI data. A sub-inventory solves the inventory

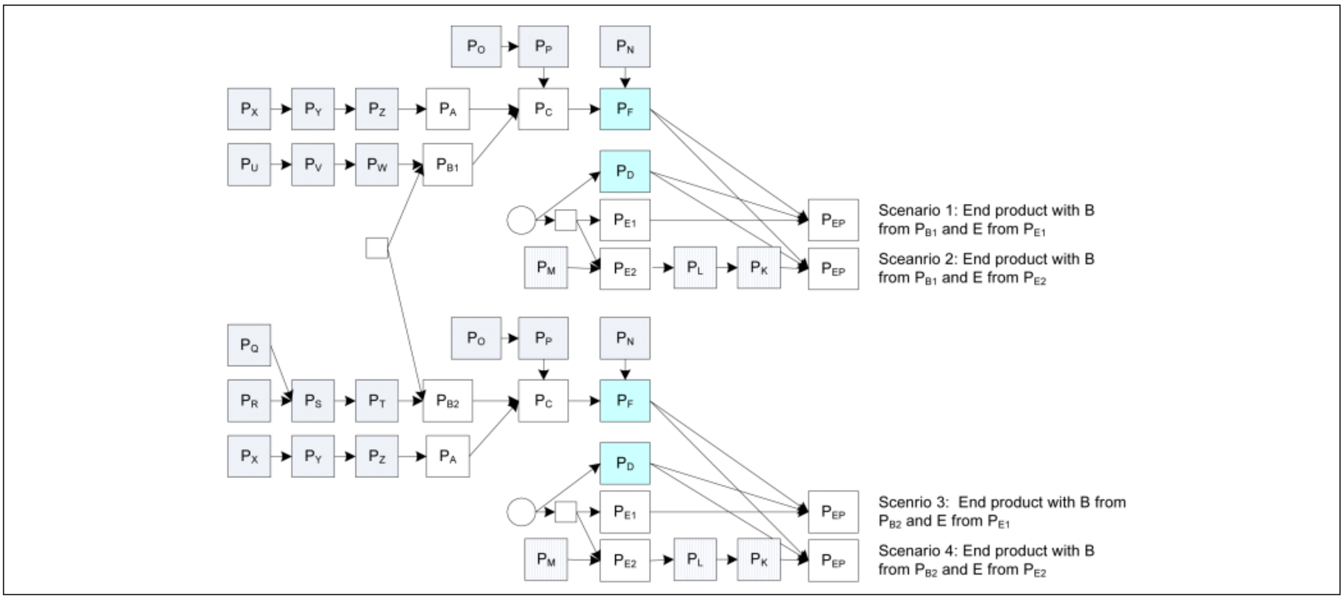

Fig. 5: Extended production system with available process decision and material chance nodes (as a process flow decision tree)

problem for sub-systems that cannot be controlled. For example, in Fig. 5 suppose sub-inventories are prepared that:

1. **Represent processes used to prepare materials with no decision nodes** (e.g., $P_X + P_Y + P_Z + P_A = P_{sA}$; $P_U + P_V + P_W + P_{B1} = P_{sB1}$; $P_Q + P_R + P_S + P_T + P_{B2} = P_{sB2}$; and $P_O + P_P + P_C = P_{sC}$; and $P_N + P_F = P_{sF}$; and in the general case cradle-to-gate commodity materials, grid electricity, and materials transport) and

2. **Represent processes preceding and following decision nodes** (e.g., $P_M + P_{E2} + P_L + P_K = P_{sE2}$) as appropriate.

As a result, the system in Fig. 5 is reduced to the same decision tree depicted in Fig. 4 with the exception that P_A is replaced by P_{sA}, P_{B1} is replaced by P_{sB1}, etc. In other words, even though the process flows in each of the processes representing sub-inventories would represent the addition of the 16 processes, the structure of the decision tree would remain the same with the same set of unique system scenarios.

The use of sub-inventories, although not codified in Heijungs and Suh [8] or elsewhere within the context of evaluating the life cycle changes for process and material alternatives, is not new. For example, when using EcoInvent [13], the practitioner can access data as either process data or as an LCI. The latter option essentially provides the practitioner with the sub-inventory. However, care must be taken to ensure that the assumptions used to prepare such an LCI or sub-inventory match that of the full LCA at hand. Given this, the data management advantages of using sub-inventories and process aggregation within decision trees are obvious for the large product systems typically evaluated in LCA.

Finally, in the same manner that decision trees can be used to estimate 'expected value' (the sum of the probability of each scenario multiplied by its 'value'), they can be used in LCA to estimate expected inventory and impact results. For example, the 'expected flow value' can be defined as:

$$EFV_{N,x} = \sum_{y} P_{N,y} s_{N,y} b_{N,x} \tag{1}$$

Similarly, when contribution to environmental impact is considered, the 'expected impact value' can be defined as:

$$EIV_{N,z} = \sum_{y} \sum_{x} P_{N,y} s_{N,y} b_{N,x} q_{xz} \tag{2}$$

where:

$EFV_{N,x}$ = the expected value of the flow x for scenario N

$P_{N,y}$ = the probability that process y will occur in scenario N, which is equal to 1 when no process alternatives are considered or the process represents an already aggregated process

$s_{N,y}$ = the scaling factor (again, the amount of each unit process needed to meet the system demand) for process y in scenario N

$b_{N,x}$ = inventory flow x (a flow to or from the environment such as bauxite, carbon dioxide emissions, etc.) for each process in scenario N

$EIV_{N,z}$ = the expected value of the contribution of the product system to impact z for scenario N

q_{xz} = the equivalency (or characterization) factor for inventory flow x for impact z

For both single branch and process flow decision trees, process scaling factors (s_y) can be estimated using the sequential method facilitated by common, iterative computing techniques and incorporated into some LCA software tools. Heijungs and Suh [8] describe the sequential method for determining the scaling factor for each unit process as starting with the end process and sequentially adding the preceding need for each upstream process as required. Although easy to understand, Heijungs and Suh note the sequential method is difficult to formalize with mathematical notation. Further, any feedback loops (such as the use of fuel to produce electricity and the use of electricity to produce fuel)

must be solved by interrupting the feedback loop after a specified number of iterations or at the point when the change in the demand is less than a specified amount, replacing the process data by data that accounts for the feedback loop, or using an infinite geometric progression.

3 Use of Disaggregated Demand Vectors

Although lacking the visual appeal of both decision tree methods and the potential use of commercially available software/ traditional decision tree solution constructs using the single branch method, disaggregation of the demand vector does not require use of the sequential method to determine scaling matrix values. However, to create formalized notation for representing process and material alternatives throughout the life cycle, disaggregation of the demand vector requires careful scenario tracking efforts. Specifically, all flows within the technosphere (in the technology and demand matrices) must be made distinguishable by the set of life cycle processes applied to them.

Fig. 6 presents an example technology matrix (a matrix of technosphere flows for the life cycle) and the associated disaggregated demand matrix. The figure continues the example in Figure 4 and uses the computational structure described by Heijungs and Suh [8] and in the introduction of this work. Again, 2 process alternatives (a choice between P_{B1} and P_{B2} and a choice between P_{E1} and P_{E2}) and 1 material alternative (a 'chance' between materials D and F) dictate a need for 4 unique system scenarios. Here, it is assumed that sub-inventories are used for the production of materials A, B, C, E2, and F (the sub-systems that are assumed cannot be controlled). Also, it has been assumed the probability that Material D will be chosen is 0.8, leaving the probability that Material E will be chosen at 0.2.

In the interpretation of Fig. 6, it should be noted that the demand vector is used to differentiate the chance between materials D and E. The technology matrix is established with 6 end products that represent the scenarios for the production of unique end products either using material D or E. Next, the probability that material D or E will be chosen is captured in the demand vector: for a system demand of 100 end products, 80 are demanded that use material D and 20 are demanded that use material E. In this way, the material alternative is evaluated without introducing multifunctional processes into the system as described above. The scaling matrix can next be used to solve the inventory problem for the 4 scenarios.

Technology Matrix (blanks represent zeros)		Production of Material A using P_{sA}	Production of Material B from P_{sB1}	Production of Material B from P_{sB2}	Production of Material C through P_{sB1}	Production of Material C through P_{sB2}	Production of Material F through P_{sB1}	Production of Material F through P_{sB2}	Production of Material D	Production of Material E from P_{E1}	Production of Material E from P_{E2}	Production of End product with D and F through P_{sB1}	Production of End product with E from P_{E1} and F through P_{sB1}	Production of End product with E from P_{sE2} and F through P_{sB1}	Production of End product with D and F through P_{sB2}	Production of End product with E from P_{E1} and F through P_{sB2}	Production of End product with E from P_{sE2} and F through P_{sB2}
Material A	kg	1			-0.4	-2											
Material B from P_{sB1}	kg	-6.55	1		-4												
Material B from P_{sB2}	kg	-1.67		1		-0.6											
Material C through P_{sB1}	kg	-2			1		-1.8										
Material C through P_{sB2}	kg					1		-1.8									
Material F through P_{sB1}	kg						1					-1.7	-1.6	-1.7			
Material F through P_{sB2}	kg							1							-1.5	-1.6	-1.7
Material D	kg	-17.6							0.8			-0.5			-0.5		
Material E from P_{E1}	kg									1			-0.6			-0.6	
Material E from P_{E2}	kg										1			-2			-1.9
End product with D and F through P_{sB1}	kg											1					
End product with E from P_{E1} and F through P_{sB1}	kg												1				
End product with E from P_{sE2} and F through P_{sB1}	kg													1			
End product with D and F through P_{sB2}	kg														1		
End product with E from P_{E1} and F through P_{sB2}	kg															1	
End product with E from P_{sE2} and F through P_{sB2}	kg																1

Disaggregated Demand Matrix		Scen. 1	Scen. 2	Scen. 3	Scen. 4
Material A	kg				
Material B from P_{sB1}	kg				
Material B from P_{sB2}	kg				
Material C through P_{sB1}	kg				
Material C through P_{sB2}	kg				
Material F through P_{sB1}	kg				
Material F through P_{sB2}	kg				
Material D	kg				
Material E from P_{E1}	kg				
Material E from P_{E2}	kg				
End product with D and F through P_{sB1}	kg	80		80	
End product with E from P_{E1} and F through P_{sB1}	kg	20			
End product with E from P_{sE2} and F through P_{sB1}	kg			20	
End product with D and F through P_{sB2}	kg		80		80
End product with E from P_{E1} and F through P_{sB2}	kg		20		
End product with E from P_{sE2} and F through P_{sB2}	kg				20

Resulting Scaling Matix	Scen. 1	Scen. 2	Scen. 3	Scen. 4
Production of Material A using P_{sA}	605	2,736	612	2,772
Production of Material B from P_{sB1}	10,009	39,809	10,129	40,333
Production of Material B from P_{sB2}	1,010	4,733	1,022	4,796
Production of Material C through P_{sB1}	1,512	5,472	1,530	5,544
Production of Material C through P_{sB2}		274		277
Production of Material F through P_{sB1}	168		170	
Production of Material F through P_{sB2}		152		154
Production of Material D	13,356	60,242	13,514	61,034
Production of Material E from P_{E1}	12	12		
Production of Material E from P_{E2}			40	38
Production of End product with D and F through P_{sB1}	80		80	
Production of End product with E from P_{E1} and F through P_{sB1}	20			
Production of End product with E from P_{sE2} and F through P_{sB1}			20	
Production of End product with D and F through P_{sB2}		80		80
Production of End product with E from P_{E1} and F through P_{sB2}		20		
Production of End product with E from P_{sE2} and F through P_{sB2}				20

Scenario 1: End product with D; E from P_{E1}; F thru P_{sB1}
Scenario 2: End product with D; E from P_{sE2}; F thru P_{sB1}
Scenario 3: End product with D; E from P_{sE2}; F thru P_{sB1}
Scenario 4: End product with D; E from P_{sE2}; F thru P_{sB2}

Fig. 6: Technology, Demand, and scaling matrices for the example product system with available process and material decisions

To prepare each sub-inventory, a process matrix is created for the sub-systems of interest as described by Heijungs and Suh [8] with two exceptions: (1) the flows within the technosphere of the sub-inventory represent those flows needed only in the sub-system (used to estimate the scaling factors for the subsystem), and (2) the economic and environmental flows for the full life cycle are treated mathematically as environmental flows (flows that leave the subsystem boundaries) in the intervention matrix and repeats the product of the sub-inventory. For example, the sub-inventory technology matrix for P_{sA} could include the production of materials X, Y, Z, and A (as in Fig. 5); the intervention matrix includes the economic and environmental flows for the full life cycle; the demand vector demands the production of material A; the scaling vector scales the sub-system processes; and the results provide economic and environmental flows for the sub-inventory to the full LCA.

The formulation presented in the example above can be used to estimate expected impact values using the exact mathematical construct presented by Heijungs and Suh [8]:

$$h_{N,i} = \sum_{j} q_{ij} g_{Nj} \qquad (3)$$

where:

$h_{N,i}$ = the contribution of the product system to impact i for scenario N

q_{ij} = the equivalency (or characterization) factor for environmental flow j for impact i

$g_{N,j}$ = components of the inventory vector for environmental flow j for scenario N

This formulation works because the probability at all chance nodes has already been accounted for in the inventory solution (i.e., by including the probability that material D or E will be chosen in the demand vector).

4 Discussion

All life cycle systems include material and process alternatives. Given this fact and noting that we are in a time of increased inventory data availability, consideration of alternatives in LCA is a critical methodological advancement. Specifically, LCAs should proceed with inventory methodologies that: (1) reveal the optimal set of processes with respect to minimization of each impact of interest while considering what decisions can and cannot be actually made, and (2) minimize and organize computational and data collection needs.

Key among the contributions here relate to process aggregation and the presentation of assessment results in scenario formulation. First is the recognition of the system reduction advantages of aggregating process alternatives but not material alternatives. The latter creates artificial multifunctional processes, and therefore creates a computational loop that does not assist in the identification of an optimal set of processes. A second key contribution is the introduction of the use of expected inventory and impact values, directly taken from decision tree computational methods. The use of expected values forces the explicit presentation of scenario results and the consideration of probabilities throughout the life cycle.

Also for scenario formulation, we note the importance and complexities of naming scenarios in a way that differentiates them from other scenarios. This is important when considering the development of LCI data for use in databases or LCA software. Although it is common to state the location of the end product and other scenario descriptors in the meta data, should data for a wide variety of alternative product systems for the same end product be entered into a database, relevant descriptors should be moved into the data set name. At a broad level, such a naming convention is already in use: the names of unit process data sets based on primary materials are commonly differentiated from those based on recycled materials. Should there be wide interest in capturing additional process and material alternatives within LCA databases, a structured and end-product-specific naming convention is needed.

Considering the usefulness of decision tree and matrix methods in scenario formulation, decision tree methods have advantages such as easily allowing the practitioner to get a visual picture of the system and the available alternatives throughout the life cycle. In addition, the decision tree methods allow interpretation of the impact of decisions early in the life cycle to be easily considered. Another advantage is that these methods allow the user to differentiate between decisions and chances and to incorporate these findings into the expected impact value. This eliminates any variables in which there is no control over the result. Despite these advantages, when looking at large systems, little is gained computationally due to the need to sequentially estimate scaling factors. Finally, once the scaling factors are estimated, decision tree software can be used with the single branch method to further assess expected inventory and impact values.

Finally, although disaggregation of the demand vector lacks the visual appeal and possible use of decision tree software of the decision tree methods, being able to estimate scaling factors without the sequential method is a clear advantage when a formal mathematical construct is desired. Although carefully naming technosphere flows and unit processes can be quite burdensome and may not be possible in some LCA software tools due to text-length limitations, given the number of unit processes typically evaluated in an LCA, this data management step is worth the effort when balanced with the ability to apply a matrix-based LCI computational structure.

5 Conclusions and Perspectives

Although LCA is frequently used for product comparison, here we recognize that improvements can be made within a product system by those capable of making such improvements. This recognition supports the greater use of LCA in supply chain formation and product research, development, and design.

In our exploration of scenario formulation and data management, we find that data collection and management are

facilitated by the use of sub-inventories (or as a complete LCI within an LCI) for process alternatives and the full consideration of material alternatives to avoid the creation of artificial multi-functional processes. We further note the importance and complexities of naming scenarios in a way that differentiates them from other scenarios. We conclude that further investigation of unit process naming conventions is needed should there be wide interest in capturing additional process and material alternatives for end products modeled within LCA databases and software.

In our evaluation of the usefulness of decision tree and matrix methods in modeling process and material alternatives, we assume that each analysis method should reveal the optimal set of materials and processes as well as minimize and organize computational and data collection needs. We conclude that although both methods are formulated herein to reveal an optimal life cycle system, because demand matrices allow the simultaneous estimation of scaling factors, we prefer its use in the communication of methodological advances based on matrix structures and in the development of LCI documentation for peer review.

The methods described here have been used in the assessment of forest management alternatives (see Sonne [14]) and are being used in two regional planning efforts. First, alternative harvest practices and end-product conversion and fabrication processes are being considered in planning the ultimate management of forest residuals in California and Washington State. Second, substitutes, recycling, trading among a variety of partners, and disposal options are being evaluated for the management of solvents in King County, Washington. We conclude that without the assessment of alternatives in these systems, we would be missing important planning opportunities for life cycle improvements.

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Life Cycle Assessment as a Tool for Improving Process Performance: A Case Study on Boron Products

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Abstract

This paper explores the use of LCA as a tool for process environmental management, thereby moving the focus from product to process oriented analysis. The emphasis is on Improvement Assessment in which the 'hot spots' in the system are targeted for maximum environmental improvements. In this context, it is useful to use multiobjective optimisation which
renders Valuation unnecessary. The approach is illustrated by the case study of the system processing boron ores to make five different products. The results of Inventory Analysis and Impact Assessment are presented and discussed. In Improvement Assessment, a number of improvement options are identified and evaluated, using system optimisation. It is shown that the site environmental performance can be improved over current operation by an average of 20% over the whole life cycle. Thus the study demonstrates that the optimisation approach to environmental process management may assist in identifying optimal ways to operate a process or plant from 'cradle to grave'. This may help the process industries not only to comply with legislation but also provide a framework for taking a more proactive approach to environmental management leading to more sustainable industrial operations and practices.

Keywords: Boron products; environmental impacts; environmental system management; system optimisation